

FIGURE 1

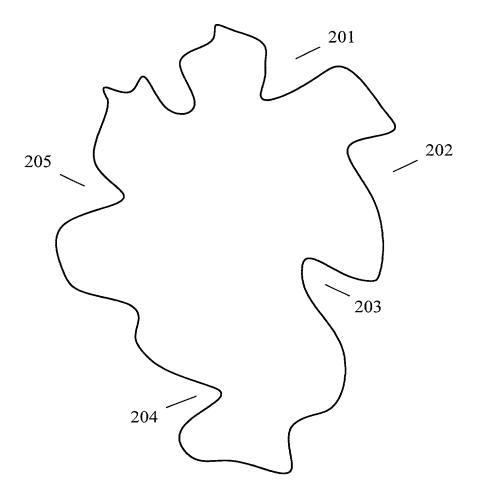
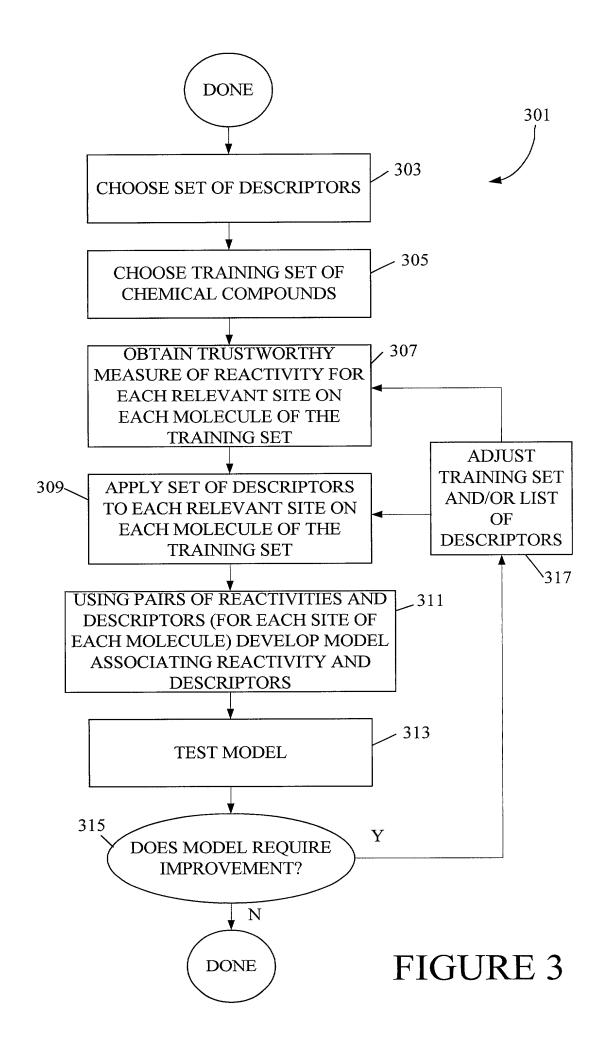


FIGURE 2



Aliphatic Model Descriptors

Charge Partial charge calculated using PEOE method

ConjSys Size of the conjugated system (aromatic + double bond systems)
ConjSysEn Total electronegativity values of immediate atom neighbors of the

conjugated system

ConjSysPC Total partial charge values of immediate atom neighbors of the

conjugated system

Fused Flag for whether the site is between fused rings

FuseStrain A strain value of the fused system

3 Ring In a 3-member ring
4 Ring In a 4-member ring
5 Ring In a 5-member ring
6 Ring In a 6-member ring

Dibenzylic Attached to two aromatic system

C Count of carbon neighbors

Aro C Count of aromatic carbon neighbors

Dbl C Count of double bonded carbon neighbors

N Count of nitrogen neighbors
 O Count of oxygen neighbors
 Si Count of silicon neighbors
 S Count of sulfur neighbors

C Ch Sum of partial charge of carbon neighbors

Aro C Ch

Sum of partial charge of aromatic carbon neighbors

Dbl C Ch

Sum of partial charge of double bonded carbon neighbors

N Ch
O Ch
Sum of partial charge of nitrogen neighbors
O Ch
Sum of partial charge of oxygen neighbors
Si Ch
Sum of partial charge of silicon neighbors
S Ch
Sum of partial charge of sulfur neighbors

Eneg Electronegativity

H Count of hydrogen neighbors

Tpl C Count of triple bonded carbon neighbors
Conj N Count of conjugated nitrogen neighbors
Aro N Count of aromatic nitrogen neighbors

Halide Count of halide neighbors

2 Neighbor
3 Neighbor
N pi
Count of neighbor atoms with 2 neighbors
Count of neighbor atoms with 3 neighbors
Count of nitrogen bonded to an sp2 atom

N E-neg Count of nitrogen bonded to an electronegative atom

Amide N Side Count of nitrogen bonded to an amide N S-Adjacent Count of nitrogen-sulfur fragment

O pi Count of fragments of oxygen bonded to an sp2 atom

Aro Ether Count of aromatic ether group
Oxy Ester Count of oxy-ester group
Oxide Count of generic oxide group

O E-neg Count of fragments of oxygen bonded to an electronegative atom S E-neg Count of fragments of sulfur bonded to an electronegative atom S 2 E-neg Count of fragments of sulfur bonded to two electronegative atom

Disulfide Count of disulfide bridges

Proximal pi Count of fragments of carbon bonded to a sp2 atom

Carboxy Count of carboxy groups

Carboxy E-neg
Count of carboxy groups bonded to an electronegative atom
Count of fragments of carbon bonded to an electronegative atom

Prox Halide Count of fragments of carbon bonded to a halide

Vinyl Carboxy
Vinyl N
Count of vinyl carboxy groups
Count of vinyl nitrogen groups
Triple Bond
Count of triple bonded carbon

Aromatic Model Descriptors

Conjug ConjugEn	Size of the conjugated system (aromatic + double bond systems) Total electronegativity values of immediate atom neighbors of the
	conjugated system
ConjugPC	Total partial charge values of immediate atom neighbors of the
	conjugated system
arC 1	Count of aromatic carbon one aromatic bond away
arC 2	Count of aromatic carbon two aromatic bonds away
arC 3	Count of aromatic carbon three aromatic bonds away
arC 4	Count of aromatic carbon four aromatic bonds away
arC 5	Count of aromatic carbon five aromatic bonds away
arC 6	Count of aromatic carbon six aromatic bonds away
arN 1	Count of aromatic nitrogen one aromatic bond away
arN 2	Count of aromatic nitrogen two aromatic bonds away
arN 3	Count of aromatic nitrogen three aromatic bonds away
arO 3	Count of aromatic oxygen three aromatic bonds away
Heavy 1	Count of neighbor heavy atom one aromatic bond away
Heavy 2	Count of neighbor heavy atom two aromatic bonds away
Heavy 3	Count of neighbor heavy atom three aromatic bonds away
E-neg 1	Count of neighbor electronegativity atom one aromatic bond away
E-neg 2	Count of neighbor electronegativity atom two aromatic bonds away
E-neg 3	Count of neighbor electronegativity atom three aromatic bonds away
C 1	Count of neighbor carbon one aromatic bond away
C 2	Count of neighbor carbon two aromatic bonds away
C 3	Count of neighbor carbon three aromatic bonds away
N 1	Count of neighbor nitrogen one aromatic bond away
N 2	Count of neighbor nitrogen two aromatic bonds away
N 3	Count of neighbor nitrogen three aromatic bonds away
01	Count of neighbor oxygen one aromatic bond away
02	Count of neighbor oxygen two aromatic bonds away
O 3	Count of neighbor oxygen three aromatic bonds away
S 1	Count of neighbor sulfur one aromatic bond away
S 2	Count of neighbor sulfur two aromatic bonds away
S 3	Count of neighbor sulfur three aromatic bonds away
pi 1	Count of neighbor sp2 atoms one aromatic bond away
pi 2	Count of neighbor sp2 atoms two aromatic bonds away
pi 3	Count of neighbor sp2 atoms three aromatic bonds away
Chg 0	Partial charge of the atom
Chg 1	Total partial charge of atoms one aromatic bond away
Chg 2	Total partial charge of atoms two aromatic bonds away
Chg 3	Total partial charge of atoms three aromatic bonds away

FIGURE 4B

Aliphatic Model Descriptor Coefficients

Descriptor	Coefficient
Const	11.03
Charge	-2.38
ConjSys	-0.05
ConjSysEn	-0.01
ConjSysPC	0.63
Fused	0.31
FuseStrain	2.80
3 Ring	2.18
4 Ring	0.94
5 Ring	0.46
	-0.53
6 Ring	0.29
Dibenzylic	
C	0.03
Aro C	-0.57
Dbl C	-0.72
N	-1.26
0	-0.01
Si	1.64
S	-0.56
C Ch	3.11
Aro C Ch	0.18
Dbl C Ch	8.43
N Ch	5.43
O Ch	0.29
Si Ch	27.40
S Ch	12.22
Eneg	-0.23
Н	0.55
Tpl C	-0.63
Conj N	0.32
Aro N	1.25
Halide	0.50
2 Neighbor	-0.17
3 Neighbor	0.17
N pi	0.11
N E-neg	-0.30
Amide N Side	0.49
N S-Adjacent	-1.07
O pi	0.43
Aro Ether	0.31
Oxy Ester	0.58
Oxide	0.89
O E-neg	1.65
S E-neg	2.44
S 2 E-neg	2.44
Disulfide	-1.46
Proximal pi	0.41
Carboxy	0.44
Carboxy Carboxy E-neg	0.31
Prox E-neg	0.32
Prox E-fleg Prox Halide	0.41
Vinyl Carboxy	1.27
	-0.77
Vinyl N	-0.63
Triple Bond	-0.03

Aromatic Model Descriptor Coefficients

Descriptor	Coefficient
Const	12.95
Conjug	-0.03
ConjugEn	-0.01
ConjugPC	0.35
arC 1	-0.86
arC 2	-0.15
arC 3	-0.27
arC 4	-0.11
arC 5	-0.03
arC 6	0.00
arN 1	0.86
arN 2	-0.46
arN 3	-0.03
arO 3	-0.42
Heavy 1	0.03
Heavy 2	0.02
Heavy 3-	0.15
E-neg 1-	0.26
E-neg 2	0.06
E-neg 3	-0.15
C 1	0.26
C 2	-0.03
C 3	-0.10
N 1	-0.26
N 2	0.05
N 3	-0.19
01	-0.31
02	-0.12
03	-0.04
S 1	0.69
S 2	-0.09
S 3	-0.46
pi 1	0.30
pi 2	0.02
pi 3	0.02
Chg 0	5.50
Chg 1	-0.89
Chg 2	1.15
Chg 3	0.29

FIGURE 5B

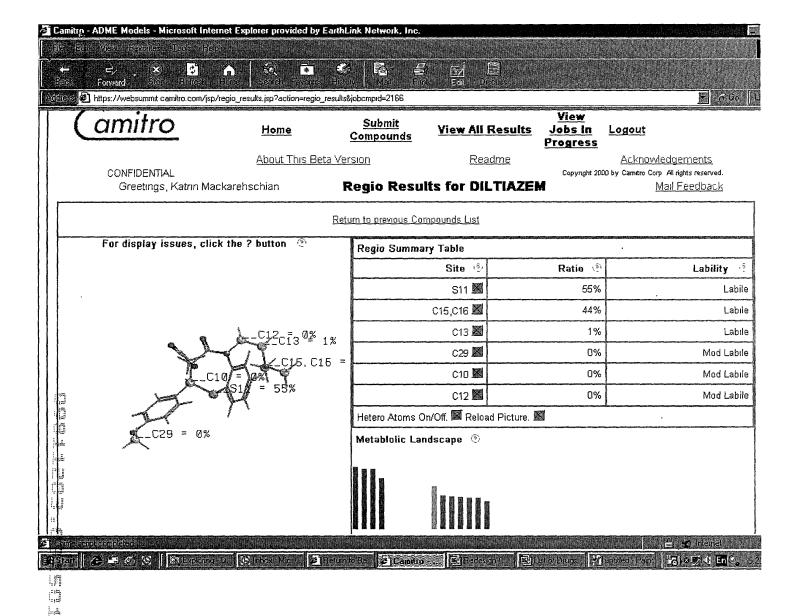


FIGURE 6

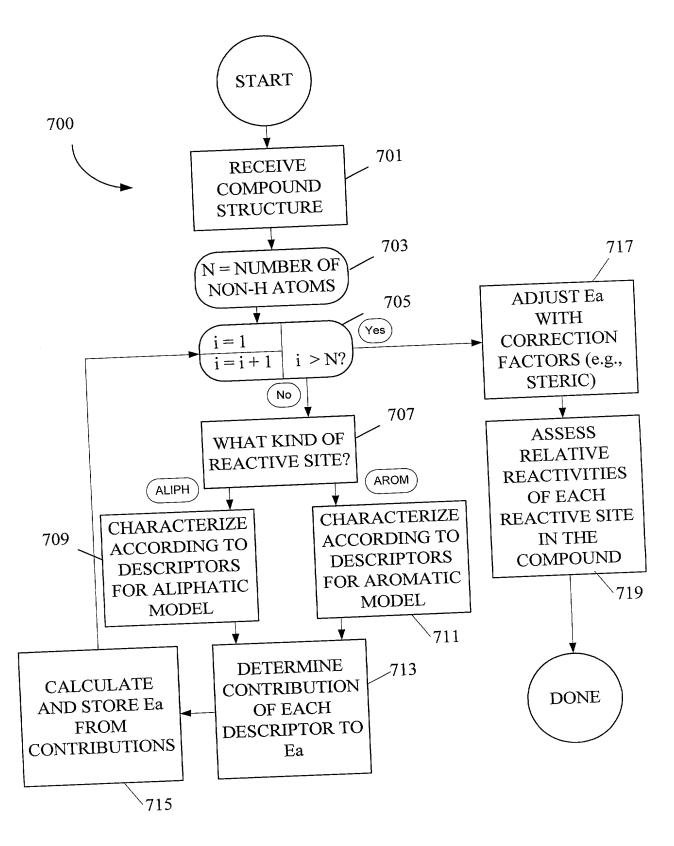


FIGURE 7

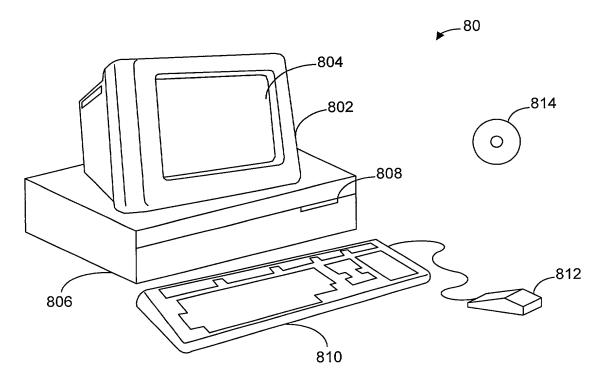


Figure 8A

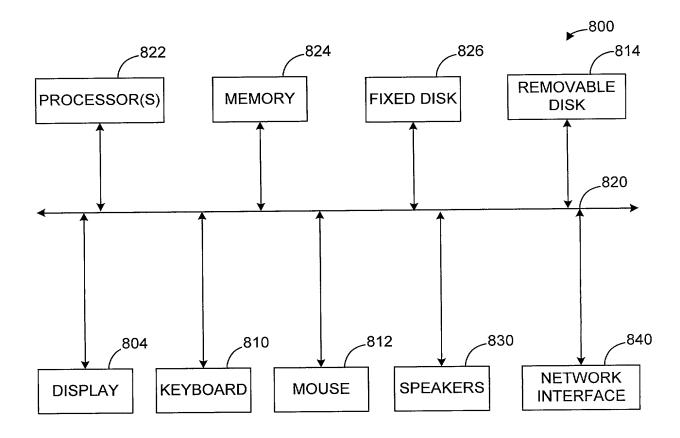


Figure 8B